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X-RAY DIFFRACTION IN LIQUIDS: ISOMERS OF NORMAL HEPTANE

G. W. STEWART

The following isomers of normal heptane were kindly supplied by the Ethyl Gasoline Corporation:

3-3, 2-2, 2-3 and 2-4 dimethyl pentane, 3 ethyl pentane, 3 methyl hexane, 2 methyl hexane, 2-2-3 trimethyl butane.

The conclusions obtained from x-ray diffraction measurements are as follows:

1. Dimethyl pentane, whether 2-3, 2-4, 2-2 or 3-3, has a greater diameter than normal heptane by 1.04Å or about twice the increase caused by two such branches in tertiary butyl alcohol, and roughly twice the increase caused by a branch CH_3 or of OH in the case of the alcohols.

2. The increase in diameter with the two CH_3 groups attached either to adjacent or nonadjacent C atoms seems to alter the diameter by the same amount, 1.04Å. This is shown by the four heptanes just enumerated.

3. The attachment of two CH_3 groups to the same atom may or may not increase the diameter by the same amount, 1.04Å, this depending upon whether a third CH_3 branch is attached to an adjacent atom (2, 2, 3 trimethyl butane or 2, 2, 4 trimethyl pentane).

4. The union of three like branches, as is 3 ethyl pentane increased the diameter by an amount indicating the probable breaking up of the "straight" chain into a symmetrical form with equal angles between each pair.

5. The area of cross-section of the molecule when the structure changes to an isomer decreases much more rapidly than computations indicate that it should. This suggests a change in the structure of the chain.

6. The paraffin molecule is a chain that is similar to but not like the alcohol chain, in that the attachment of side branches does not indicate equal alterations in diameter.

7. The structure of 3 methyl hexane is better termed 2 ethyl pentane.

8. The attachment of a CH_3 group on the next to the end C atom evidently alters the end of the chain, causing a symmetrical arrangement of the two CH_3 groups and increasing the diameter of the molecule by a relatively small amount.

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